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## FINAL REPORT

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### EIGENVECTORS of GRAPHS

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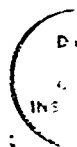
## ABSTRACT

→ This grant has supported work in several areas.

1. A study of graph eigenvectors shows connections to graph structure in ways that are reminiscent of eigenfunctions of the laplacian operator in two or three dimensions. Methods developed in this study have also led to estimates of the maximum possible value for the  $k$ th eigenvalue of a graph as function of the number of edges or vertices.

2. The convex hull of the rows of an eigenmatrix of a graph is the polytope of an eigenvalue. We investigated relations between such polytopes and the graph. The graph of such a polytope may be isomorphic to the original graph: this is the case for most regular polytopes. For distance regular graphs and several kinds of less symmetric graphs, we can show that the polytope of some eigenvalue has the same group of automorphisms as the graph, that proximity of points is equivalent to adjacency of vertices, and that other properties of the polytope carry over to the graph.

Possible directions for future work include the following. Determine the reducibility of the group of automorphisms of a polytope and the significance in the graph of faces and facets of the polytopes. Investigate the intrinsic eigenvectors of a graph (the list of inner products of vertices of a polytope with the normal to a supporting hyperplane is an intrinsic eigenvector). Seek physical models for the interpretation of graph eigenvalues and eigenvectors, e.g., transient temperature distributions in a graph-like collection of heat-conducting rods.



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## 1. WORK SUPPORTED BY THIS GRANT

### A. Journals and Reviewed Proceedings

[1] Structure of a matrix according to its second eigenvector. In Current Trends in Matrix Theory, F. Uhlig and R. Grone, eds. North-Holland, New York/Amsterdam, 1987, pp. 261-266.

[2] A surprising property of some regular polytopes. *Scientia* (Valparaiso), Festschrift for R. Frucht. (With C. Licata.) To appear.

[3] Graph partitioning by eigenvectors. *Linear Algebra and Applications* (101) 1988, pp. 121-133.

[4] Eigenvectors of distance-regular graphs. *SIAM J. Matrix Analysis and Applications* (9) 1988, pp. 399-407.

[5] Semiregular graphs and their algebra. *Linear and Multilinear Algebra*. To appear.

[6] Bounds on graph eigenvalues. *Linear Algebra and Applications*. To appear.

[7] Partially distance-regular graphs. In Proceedings of the Sixth International Conference on the Theory and Applications of Graphs, G. Chartrand and A. Schwenk, eds. To appear.

### B. Technical Reports

[8] Graph eigenvectors. Clarkson University, 1986.

[9] Tree eigenvectors. Clarkson University, 1986.

[10] The Petersen polytopes. Clarkson University, 1986.

### C. Presentations

Structure of a matrix according to its second eigenvector. International Matrix Theory Conference, Auburn AL, March 1986.

Structure of a weighted graph according to its eigenvectors. SIAM Conference on Linear Algebra, Boston MA, August 1986.

Graphs and matrices. Conference on Combinatorics and Graph Theory, Oswego NY, October, 1986.

Graph eigenvectors and polytopes. MAA Summer Seminar on Linear Algebra and Graph Theory, Duluth MN, June, 1987.

Partially distance-regular graphs. Sixth International Conference, Theory and Applications of Graphs, Kalamazoo MI, May-June, 1988.

## 2. REVIEW OF WORK DONE

### A. Eigenvectors and Spectrum Relative to Graph Structure

Notation. In the following,  $G$  is a connected graph with vertex set  $V = \{1, 2, \dots, n\}$  and adjacency matrix  $A$ . A column matrix of 1's is denoted by  $e$ , and  $e_i$  is the  $i$ th column of an identity matrix. The eigenvalues and eigenvectors of  $G$  are those of  $A$ .

If  $z$  is any  $n$ -vector -- especially, an eigenvector of  $A$  -- we speak of a vertex of  $G$  being positive, negative, zero, etc., accordingly as the corresponding entry  $z_i$  has that property. Fiedler (1975) proved the following theorem.

Theorem. Let  $z$  be any eigencolumn of  $G$  associated with the second eigenvalue  $a$  of  $G$ . The nonnegative vertices induce a connected subgraph of  $G$ .

In [1] we studied the role of the zero vertices in Fiedler's theorem, arriving at the following sharpening of his result.

Theorem 1. Let  $a$  be the second eigenvalue of  $G$  with multiplicity  $m$ , and let  $z$  be an eigencolumn of  $G$  associated with  $a$ . Assume that the  $i$ th entry of  $z$  is zero iff the  $i$ th entry is zero in every eigenvector associated with  $a$ . One of the following holds. (1) The zero vertices are a disconnecting set, and the nonzero vertices induce a subgraph of  $G$  with  $m + 1$  connected components. The first eigenvalue of each of the components is  $a$ . (2) The zero vertices are not a disconnecting set, and connected subgraphs of  $G$  are induced by the positive vertices, the negative vertices or the nonzero vertices. The first eigenvalue of the graphs induced by the positive or negative vertices is greater than  $a$ .

This theorem, like Fiedler's, is stated in more general terms in the paper than here. Case (1) of the theorem when  $m = 1$  resembles the situation of the Laplacian operator with Dirichlet conditions on a plane region  $R$ . Suppose that  $u(x, y)$  is an eigenfunction of the Laplacian associated with  $a$ , the second eigenvalue (counting from least up). Then the subregion  $P$  where  $u$  is positive is connected and  $a$  is the least eigenvalue of the Laplacian on  $P$  with Dirichlet conditions.

In [3] we carried this kind of analysis further, generalizing Theorem 1 above as follows.

Theorem 2. Let  $z$  be an eigenvector of  $G$  associated with an eigenvalue  $a$  of multiplicity  $m$ , and let  $t > 0$  be the number of eigenvalues greater than  $a$ . Assume that  $z_i$  is 0 if and only if the  $i$ th entry is zero in every eigenvector associated with  $a$ . One of the following holds. (1) The zero vertices are a disconnecting

set, and the nonzero vertices induce a subgraph with  $k$  components, where  $m + 1 \leq k \leq m + t$ . (2) The zero vertices are not a disconnecting set, and the nonzero vertices induce a subgraph with  $k$  components, where  $k \leq m + t - 1$ .

The ideas of this theorem led to several bounds on eigenvalues that are best possible.

Theorem 3. Let  $a$  be the second and  $-b$  the least eigenvalue of  $G$ . Then  $a \leq [(n-2)/2]$ ; the bound is achieved if  $n$  is odd and is asymptotically sharp if  $n$  is even. Also  $b \leq \sqrt{n^2 - 1}/2$  for  $n$  odd or  $b \leq n/2$  for  $n$  even; both bounds are achieved.

Corollaries of this theorem bound the first and second eigenvalues of bipartite graphs and the multiplicity of an eigenvalue in terms of its magnitude.

Historically, studies of eigenvalues have focussed on their value -- e.g., on the magnitude of the largest eigenvalue of the adjacency matrix, or the second eigenvalue of the laplacian matrix. However, the distribution of eigenvalues must also contain information, and in this regard it is useful to have absolute bounds on the  $k$ th eigenvalue. Let  $a_k(n)$  be the maximum value that can be attained by the  $k$ th eigenvalue of a connected graph on  $n$  vertices, and let  $b_k(q)$  be the maximum value that can be attained by the  $k$ th eigenvalue of a connected graph on  $q$  edges. In [6] we develop these estimates on  $a$  and  $b$ , for  $k \leq n/2$ :

$$\begin{aligned} & n/k - 1 \text{ (if } k \text{ divides } n) \\ [(n-1)/k] - 1 \leq a_k(n) \leq & \lfloor n/k \rfloor \text{ (if } k \text{ does not divide } n) \end{aligned}$$

$$b_1(\lfloor q/k \rfloor - 1) \leq b_k(q) \leq \sqrt{2(q-k)/k}.$$

The last bound assumes  $n \geq q$ . The function  $b_1(q)$  has recently been determined by Rowlinson (1988) as the largest root of a cubic. Note that the difference between the upper and lower estimates is bounded and not large.

## B. Self-reproducing Polytopes

Let  $a$  be an eigenvalue of  $G$  with multiplicity  $m$ . A matrix  $Z$  is a complete eigenmatrix associated with  $a$  if  $AZ = aZ$ ,  $Z^T Z = I_m$ . Godsil (1978) suggested constructing the polytope  $C(a)$  that is the convex hull of the points in  $m$ -space whose coordinate matrices are the rows of  $Z$ :  $w_i^T = e_i^T Z$ ,  $i = 1, 2, \dots, n$ . If  $P$  is a  $d$ -polytope, its skeleton,  $\text{skel}(P)$ , is the graph formed by its extreme points or 0-faces as vertices and its lines or 1-faces as edges. If  $P$  is isomorphic to a polytope  $C(a)$  associated with the eigenvalue  $a$  of  $G = \text{skel}(P)$ , we say that the polytope is self-reproducing.

Computer-graphic experiments indicated that many familiar polyhedra, including the regular and semi-regular polyhedra with up to 30 points, are self-reproducing (Fig. 1). In [3] we proved the following by essentially ad-hoc methods.

Theorem 4. The following regular polytopes are all self-reproducing: polygons; Platonic solids; simplexes; cross polytopes; orthotopes.

There are continuous analogs of the self-reproducing polytopes. For example, let  $S$  be the unit sphere centered at the origin. It is known -- see, e. g., Chavel, 1984, p. 35 -- that the coordinate functions are eigenfunctions of the laplacian operator corresponding to the second (counting up from the least) eigenvalue. That is, each of the functions  $u_1, u_2, u_3$  given by

$$[u_1(\theta, \phi), u_2(\theta, \phi), u_3(\theta, \phi)] = [\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta]$$

satisfies  $\Delta u = 2u$  on  $S$ . Now, as  $(\theta, \phi)$  ranges through  $[0, 2\pi] \times [0, \pi]$ , the point whose rectangular coordinates are  $u_1, u_2, u_3$  ranges over the sphere  $S$ .

We have been able to use this fact to prove that the regular polyhedra are self-reproducing, by integrating a linear combination of  $u_1, u_2, u_3$  over suitable regions of  $S$ .

Attempts to characterize self-reproducing polytopes have not yet been successful. Another approach is to look for graphs  $G$  for which  $\text{skel}(C(a))$  is isomorphic to  $G$ , so that  $C(a)$  is self-reproducing. An obvious necessary condition for  $C(a)$  to be self-reproducing is that the rows of  $Z$  be distinct.

As a starting point, we investigated distance-regular graphs [3], because they have convenient algebraic properties.

#### C. Eigenvectors and Polytopes of Distance-regular Graphs

Definition: A partition of the vertex set of a graph  $G$  into  $V_1, V_2, \dots, V_t$  is a coloration if, for any  $i$  and  $j$ , each vertex  $h$  in  $V_i$  is adjacent to the same number,  $b_{ij}$ , of vertices in  $V_j$ . The square matrix  $B = [b_{ij}]$  is called the coloration matrix of the partition.

A matrix-theoretic definition is this. Let  $X$  be the incidence matrix of the partition; that is,  $X$  has a 1 in the  $i,j$ -position if vertex  $i$  is in  $V_j$  or a 0 otherwise. Then the partition is a coloration if and only if  $AX = XB$  for some  $B$ , where  $A$  is the adjacency matrix of the graph. If the condition is fulfilled, then  $B$  is in fact the coloration matrix. Note that every row of  $X$  is a row of the identity, and no column is zero; thus  $X$  has independent columns. A general reference for colorations is Cvetkovic et al.(1980).

Definition: A graph  $G$  is distance-regular if, for each vertex  $i$  of  $G$ , the distance partition starting at  $i$ ,  $V_1 = \{i\}$ ,  $V_k = \{j: \text{dist}(i,j) = k-1\}$ , is a coloration, and the coloration matrix  $B$  is independent of  $i$ . A reference for distance-regular graphs is Biggs (1974).

Theorem 5. Let  $G$  be a distance-regular graph,  $a$  its second eigenvalue,  $Z$  a complete eigenmatrix. Then the rows of  $Z$  are distinct. (Godsil (1987) has shown that this theorem holds for an eigenvalue  $a$  if the number of distinct eigenvalues greater than  $a$  is odd.)

Using this theorem, we proceed to obtain information about the automorphism group of  $G$ . First, we define the group (See Coxeter, 1973, p. 253.) of orthogonal matrices that preserve the rows of  $Z$  setwise:  $\text{orth}(Z) = \{R: ZR = PZ \text{ for some permutation } P\}$ .

Theorem 6. Under the hypotheses of Theorem 5,  $\text{orth}(Z)$  is isomorphic to the automorphism group of  $G$ .

As a corollary, one sees that the group of automorphisms of  $G$  has a representation as a subgroup of the orthogonal group of degree  $m = \text{multiplicity of the second eigenvalue}$ . We conjecture that this representation is irreducible. This corollary sharpens results of Babai (1978) and Godsil (1978).

Theorem 7. Under the hypotheses of Theorem 5, two vertices  $i$  and  $j$  are adjacent in  $G$  iff the distance between the corresponding points  $w_i^T$  and  $w_j^T$  is minimal.

Thus the mapping between  $G$  and  $C(a)$  transforms adjacency into proximity. Godsil (1987) uses this theorem (proved independently by him) to show that a distance-regular graph with valency at least 3 is planar iff the second eigenvalue has multiplicity 3.

Further results are obtained in [4] for graphs that are antipodal: for each vertex, there is exactly one vertex at distance  $d = \text{diameter of } G$ .

In thinking about the convex hull of the rows of  $Z$ , it is natural to consider a vector of the form  $Zu = f$  as a list of inner products of rows of  $Z$  with  $u$ :  $f_i = w_i^T u$ . The vector  $u$  is normal to a facet ( $f$  is then called a facet vector) if and only if: (1) there is a number  $c$  such that  $f_i \leq c$  for all  $i$ ; (2) equality holds for at least  $m$  values of  $i$ , and the corresponding rows of  $Z$  have rank  $m$ . These latter rows are the points of  $C(a)$  that lie on the facet. A facet vector is an eigenvector of  $G$  that is independent of the matrix  $Z$  used to find it; thus it contains information intrinsic to the graph  $G$ .

Using facet vectors, it is shown in [4] that the points corresponding to the neighbors of a vertex cannot all lie on the same facet of  $C(a)$ . Also it can be shown that  $G$  is a subgraph of the skeleton of  $C(a)$ .

#### D. Eigenvectors and Polytopes of Other Graphs

In [5] the results above are extended to a broader class. A bipartite graph is semiregular if, for one of the partite sets  $V'$ , the distance partition starting at vertex  $i$  in  $V'$  is a coloration, and the coloration matrix  $B$  is independent of  $i$ . Thus,  $G$  "looks like" a distance-regular graph from each vertex in  $V'$ . This class includes the class called distance-regularized by Godsil and Shawe-Taylor (1987). The following theorem extends well known results for distance-regular graphs.

**Theorem 8.** Let  $G$  be a semiregular graph with diameter  $d$ . Then  $G$  has  $d + 1$  distinct eigenvalues. The nonzero eigenvalues of  $G$ , their multiplicities and the associated eigenvectors are determined by  $B$ .

It was also possible to extend Theorems 5 and 6 to the broader class, although extra hypotheses were needed to compensate for the weaker structure.

**Theorem 9.** Let  $G$  be a semiregular graph and  $Z$  be a complete eigenmatrix associated with the second eigenvalue  $a$ . Then the rows of  $Z$  are distinct iff no two vertices have all their neighbors in common. (Two vertices with all neighbors in common are called equivalent.)

**Theorem 10.** Let  $G$  be as in Theorem 9, and let  $G$  have no equivalent vertices. Then  $\text{orth}(Z)$  is isomorphic to the automorphism group of  $G$  if (1) the valencies of vertices in the two partite sets  $V'$  and  $V''$  are different, or (2) the automorphisms of  $G$  are transitive on  $V''$ .

In [7] we broaden the target to the class of arc-transitive graphs in this way. Select a vertex  $k$  and partition the vertices into the orbits of the stabilizer of  $k$ :  $V_1 = \{k\}$ ,  $V_2 = \{j: j \text{ adjacent to } k\}, \dots, V_t$ . (Note that in a distance-transitive graph, this partition is just the distance partition starting at  $k$ , and  $t = 1 + \text{diameter of } G$ .) This partition is a coloration with coloration matrix  $B$ . Next we use the automorphism group to establish a relation  $R_h$  on the vertices for each  $h = 1, 2, \dots, t$ :  $(i, j)$  is in  $R_h$  if there is an automorphism  $g$  of  $G$  such that  $g(j) = k$  and  $g(i)$  is in  $V_h$ . About the matrices  $A_h$  of these relations, we know that  $A_1$  is the identity and  $A_2$  is the adjacency matrix  $A$  of  $G$ , but in general these matrices are not symmetric. The following generalize well known theorems about distance-regular graphs.

**Theorem 11.** The vector space generated by  $A_1, A_2, \dots, A_t$  includes the algebra of polynomials in  $A$ .

**Corollary.** An arc-transitive graph has at most  $t$  distinct eigenvalues.

**Theorem 12.** The eigenvalues of  $G$ , their multiplicities and the associated eigenvectors are determined by  $B$ .



For a distance-regular graph, the triangle inequality forces the coloration matrix to be tridiagonal. This special property allows us to prove lemmas about the eigenvectors of  $B$  upon which the proofs of Theorems 5-7 are built. The structure of the coloration matrix  $B$  for an arc-transitive graph is much more complicated; instead of proving lemmas about its eigenvectors, we must make assumptions about them as additional hypotheses for the theorems.

### 3. FUTURE DIRECTIONS

#### A. Vector Representations of a Graph.

Recently, Parsons and Pisansky (1987) have investigated vector representations of a graph: mappings from the vertices to points in a vector space that somehow preserve adjacency and nonadjacency. Clearly the one-to-one representation by rows of an eigenmatrix, mentioned above, is one example. If the convex polytope formed on these has significance for a graph, then the sets of graph vertices that map into extreme points of faces or facets must also play a special role in the structure of the graph, perhaps in much the same way that they do in polyhedral graphs. We know, for instance, that girth-cycles map into faces and edges map into 1-faces in the case of a distance-regular graph (second eigenvalue). Vice-versa, in the polytope corresponding to the second eigenvalue of the Petersen graph, the extreme points of facets are images of the vertices of 5-cycles and 6-cycles. One would expect the preimage of a facet to be a connected and perhaps distance-preserving subgraph, at least.

#### B. Intrinsic Eigenvectors.

Suppose  $C(a)$  is the polytope associated with eigenvalue  $a$  of a walk-regular graph (i.e., such that every power of  $A$  has uniform diagonal, so all rows of a complete eigenmatrix have the same euclidean norm). Then for each facet of  $C(a)$  there is a facet vector, which is also an eigenvector. These facet vectors have some promising properties which suggest the name of intrinsic eigenvectors. In particular, they span the space of eigenvectors and contain all the point-facet incidence information, thus providing a complete combinatorial description of the polytope and its dual as well. It is reasonable to look to these vectors for a link between the geometric and algebraic aspects of a graph.

#### C. Reducibility of the Representation of $\text{Aut}(G)$ .

We have shown that the symmetry group of the rows of a complete eigenmatrix for the second eigenvalue is isomorphic to the automorphism group of  $G$  for distance-regular, semiregular, and some arc-transitive

graphs. It is desirable to know conditions under which this representation is irreducible. We know, for instance, that the representation is irreducible for many polytopal graphs, and that a necessary condition for irreducibility is automatically met. Understanding of reducibility of the representation would also provide new insight into the significance of eigenvalue multiplicity and connections to some other parameters such as diameter and girth, at least for highly symmetric graphs.

#### D. Heat Conduction on Graphs

One way to understand the significance of graph eigenvalues is to find a dynamic physical system in which they play a role. For example, Maas (1987) proposes a graph as a model of a system of pipes; flow of a suitable fluid in the pipes is then related to the eigenvalues of the laplacian matrix of the graph. A promising alternative is to take a graph as a model of a collection of insulated rods. Then the transient temperature distribution in the rods will lead to a (continuous) eigenvalue problem that is related to a matrix eigenvalue problem. The solution of this heat problem should provide a format for interpreting some graph eigenvalues.

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